Building scheme for IMF

1. Periodic Building Unit:

IMF can be built using units of 36 T atoms built from three different sub-units of 12 T atoms each (one T36-unit bold Figure 1). All three T12-units consist of two 5-1 units which are connected into a $[4^1 5^4 6^1]$-cage attached to a single T atom (T12-unit1), or into $[5^4]$- and $[5^2 6^1]$-cages (sharing a 5-ring) bearing a dimer (T12-unit2) or two single T atoms (T12-unit3). T36-units, related by a screw rotation of 180º about **b** are connected into chains along **b**. Chains, related by a screw rotation of 180º about **a** are connected along **a** into the Periodic Building Unit (PerBU). The two-dimensional PerBU equals the **ab** layer shown in Figure 1.
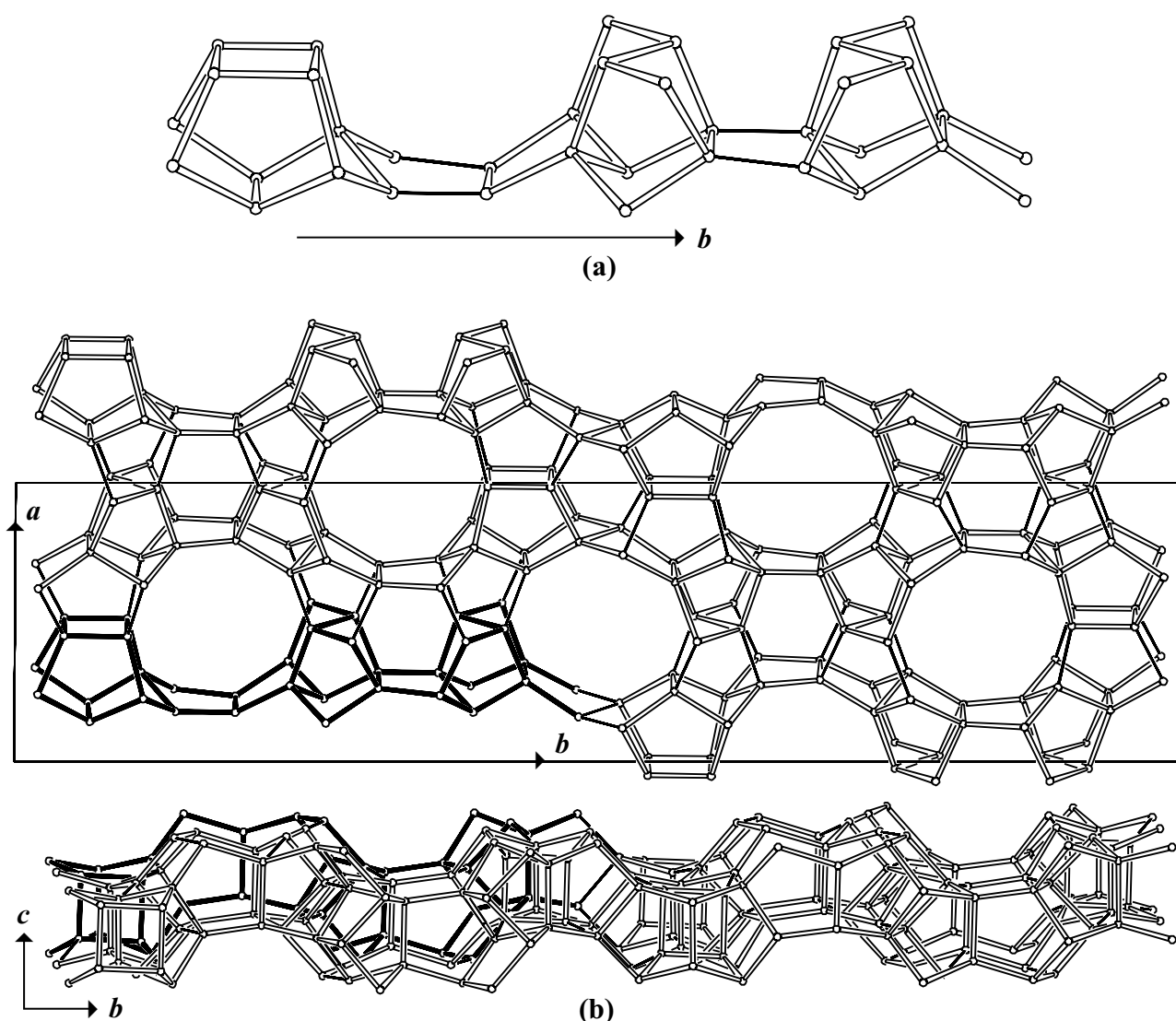

Figure 1. (a): T36-unit consisting of three different T12-units; (b): PerBU viewed along **c** (top) and along **a** (bottom).

2. Connection mode:

Neighboring PerBUs, related by a rotation of 180º about *c*, are connected along *c* as depicted in Figure 2.
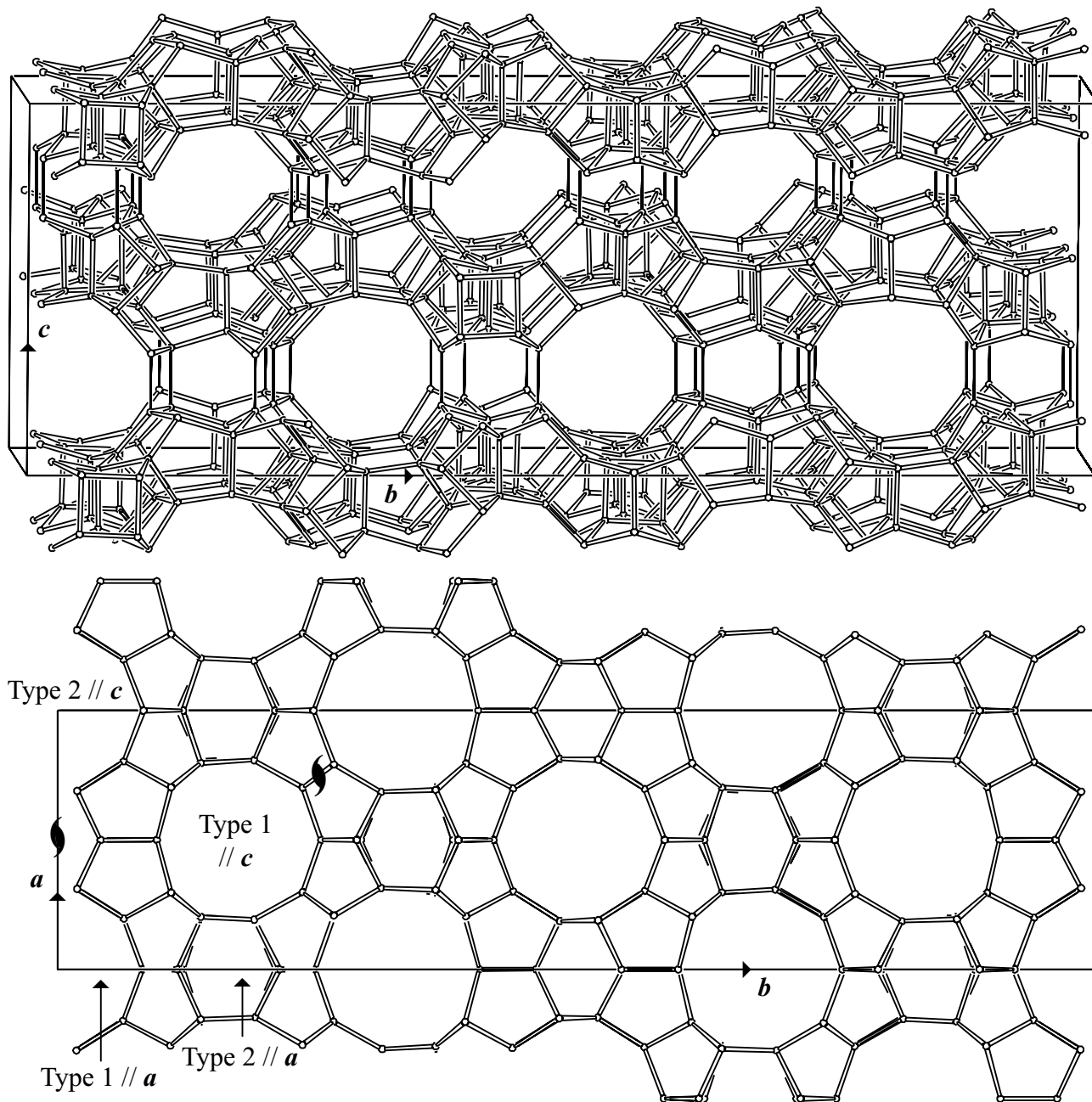

Figure 2. Top: connection mode (and unit cell content) viewed along *a*. Bottom: projection of the unit cell content along *c*. The position of 2-fold screw axes and the different types of 10-ring channels parallel to *a* and *c* are indicated (see Figure 3(b))).

3. Projections of the unit cell content: See Figure 2.

▲

4. Channels and/or cages:

There are two types of intersecting 10-ring channels parallel to *c* and parallel to *a* as indicated in Figure 2 and as illustrated in Figures 3(a) and 3(b). The **pore descriptors** are added. Pairs of 10-ring channels (of different type) parallel to *c* are interconnecting along *b* through channels of type 1 parallel to *a* as shown in Figure 3(c). The interconnecting range along *b* is limited to a slab formed by two pairs of channels, related by a 2-fold screw axis parallel to *c*.
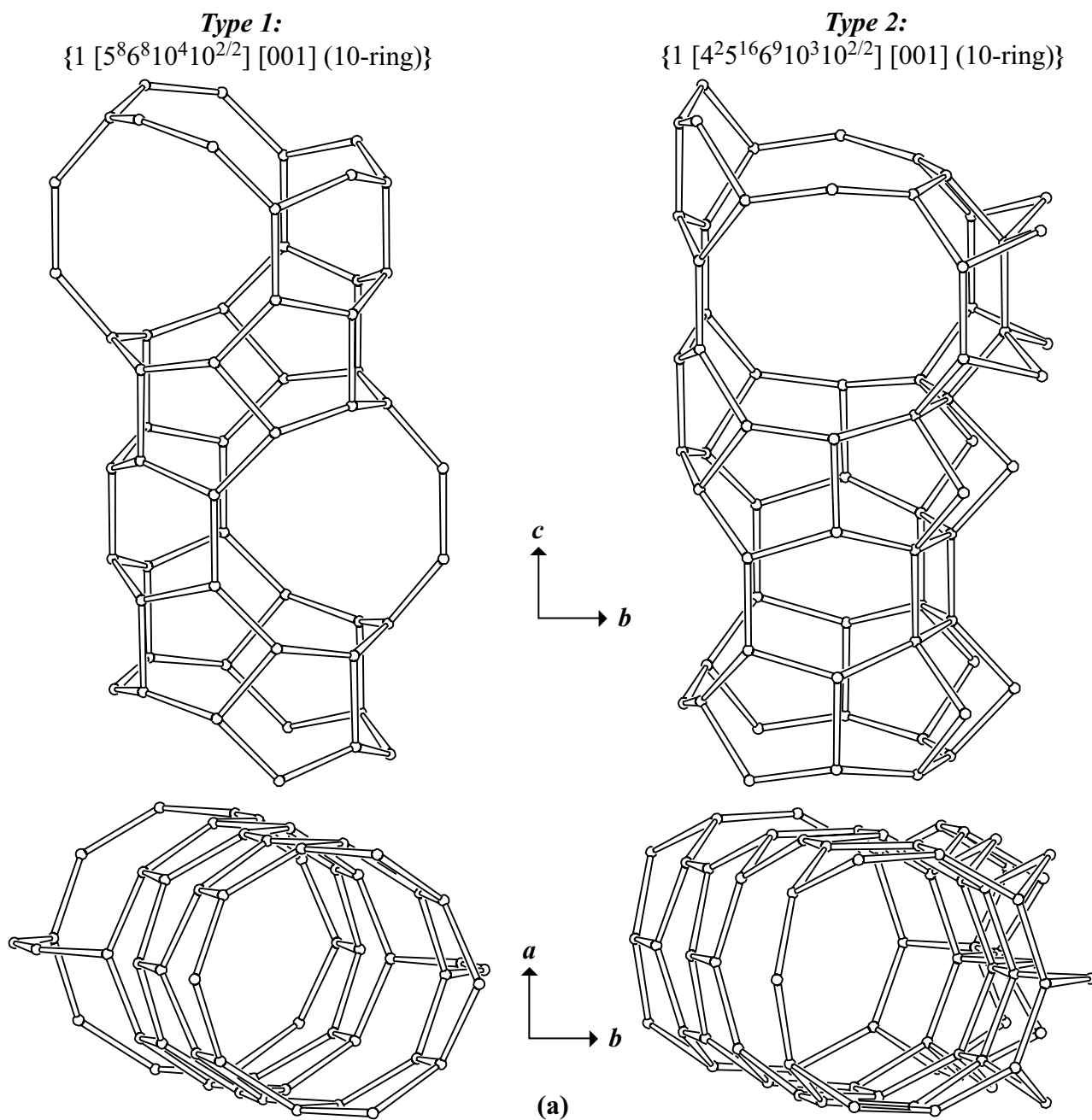
Type 1:
{1 [$5^8 6^8 10^4 10^{2/2}$] [001] (10-ring)}

Type 2:
{1 [$4^2 5^{16} 6^9 10^3 10^{2/2}$] [001] (10-ring)}

(a)

Figure 3. (a): 10-Ring channels parallel to *c* viewed along *a* (top) and along the channel axis parallel to *c* (bottom). [Figure 3 is continued on next page]
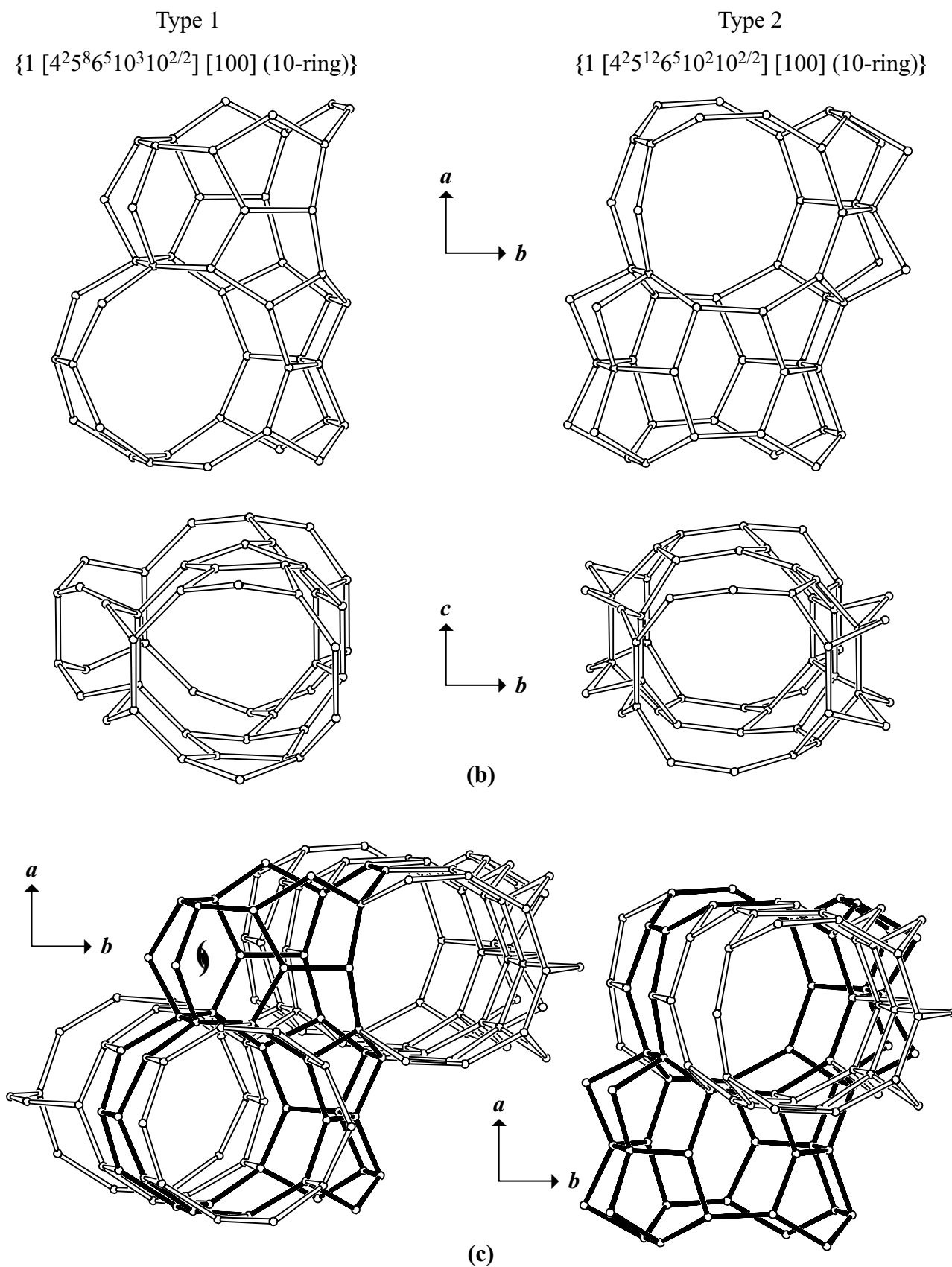
Type 1

$\{1 \ [4^2 5^8 6^5 10^3 10^{2/2}] \ [100] \ (10\text{-ring})\}$

Type 2

$\{1 \ [4^2 5^{12} 6^5 10^2 10^{2/2}] \ [100] \ (10\text{-ring})\}$

(b)

(c)

Figure 3 [Cont'd]. (b): 10-Ring channels parallel to *a* viewed along *c* (top) and along *a* (bottom). (c): Left: two types of channels parallel to *c* are interconnecting along *b* through channels of type 1 parallel to *a*. Right: Intersecting channels of type 2.

5. Supplementary information:

Other framework types containing (modified) 5-rings

5-Rings can be connected in several other ways. In all cases additional T atoms are needed to build the framework.

In the **INTRO**-pages links are given to a detailed description of a sub-set of framework types that contain (modified) 5-rings (choose: **5-Rings**). There is also a link provided to a summary of the PerBUs used in the building schemes of these framework types (choose: **Appendix**; **Figure 6**).